

(O,1,1,1,2,3,3,3-2H8)Propan-2-ol
22739-76-0 | DTXSID30177279

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 9.46 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.60e-01

Confidence level: 6.67e-01

Nearest Neighbors from the Training Set

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Isopropanol

Measured: 16.6

Predicted: 9.46

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1-Propanol

Measured: 16.6

Predicted: 13.1

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Methallyl alcohol

Measured: 2.69

Predicted: 6.51

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2-Methyl-1-propanol

Measured: 1.15

Predicted: 1.50

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But-2-en-1-ol

Measured: 13.9

Predicted: 6.02